# Experimental quantification of the energy landscape of complex systems by hyperquenching studies

Angell, C. A.; Yue, Yuanzheng; Wang, L-M.; Copley, J. R. D.; Borick, S.

*Publication date:*
2002

*Document Version*
Accepted author manuscript, peer reviewed version

# Experimental quantification of the energy landscape of complex systems by hyperquenching studies.

C. Austen Angell*, Yuanzheng Yue[#], Limin Wang*, John R. D. Copley[@] and Steve. Borick[±]

*Dept. of Chemistry and Biochemistry, Arizona State Univ., Tempe, AZ85287
[#] Danish Center for Materials Technology, Aalborg University, 9220 Aalborg, Denmark
[@] National Institute of Standards and Technology, Gaithersburg, MD 20899-8562
[±] Scottsdale Community College, Scottsdale, AZ 85256-2626

The "energy landscape" has provided an important conceptual route to dissecting the properties of liquids into separate quasi-independent contributions, namely those due to structure and those due to vibrational dynamics. Thus the system is thought of as being characterized by two temperatures, a fictive temperature $T_f$ that relates to potential energy and a real temperature that relates to kinetic energy. When the two temperatures are the same, the system is a liquid. Otherwise it is a glass.

The division depends on the different time scales for vibration and relaxation that characterize viscous liquids. Accordingly it is possible to trap the liquid in different states of configurational excitation and then to study the effect of inherent structure energy (or level on the landscape) on the vibrational dynamics. We use hyperquenching methods (melt spinning of mineral glasses and electrospray quenching of molecular glasses), to cool liquids ten million times faster than normal, and thus trap them in states approaching the mode coupling theory $T_c$, now called the crossover temperature (i.e. approaching the slowest cooled "computer glass" state).

By annealing the trapped structure, i.e. by allowing the system to escape from its initial trap in a controlled manner, one can study both relaxational dynamics and the vibrational dynamics at different levels of the landscape. Here we show, using cold neutron inelastic scattering, how the higher landscape levels are characterized by greatly increased populations of low frequency modes at the boson peak frequency. This yields a distinct ~30 $cm^{-1}$ peak in the DOS. We will suggest that this is a defect signature. Using differential scanning calorimetry we show these higher level traps are of decreasing trap depth, and determine their energy excess over that of the "standard glass",(one formed by cooling at 0.33K/s). We also find that a single fictive temperature is inadequate to describe the trapped system. Relative to the standard glass some "parts" of the hyperquenched glass relax more slowly and other parts relax more quickly. This demonstrates that the system is more complex than the usual "single system point moving on the 3N + 1 dimensional energy hypersurface " description suggests. It also

demonstrates that the much-studied dynamic heterogeneity has a potential energy (hence structural) manifestation. Comparisons will be made with simulations of orthoterphenyl in different structural states, obtained by Mossa et al.